Advancing our Understanding Materials and Achieving Exascale Supercomputing is Critical to the Future of Los Alamos

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LDRD Day

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Los Alamos provides science and engineering solutions to the Nation's security issues

- **Stockpile Stewardship is core mission**
- **Lab's tools also address other national priorities**
- **Technologies to reduce national security threats**
- **Solutions to challenges of energy security**

"…science holds the key to our survival as a planet and our security and prosperity as a Nation. It's time once again to put science at the top of our agenda and work to restore America's place as world leader in science and technology." President Obama

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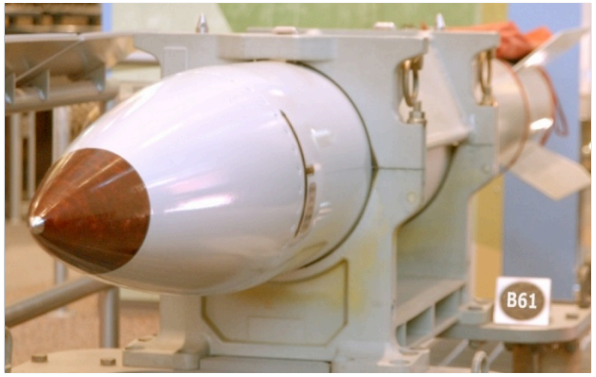
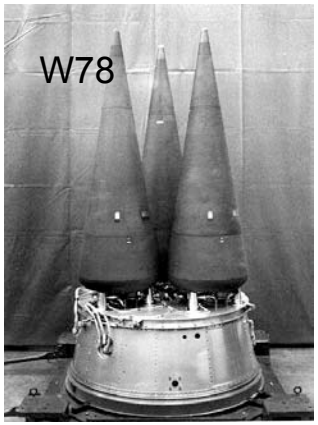
Sustaining the nuclear deterrent over the long term requires investing in leading edge science and technology

- LANL is the design laboratory for:
  - W76 SLBM
  - W88 SLBM
  - B61Gravity bomb
  - W78 ICBM
- Requires the best science and engineering (people and technology)





" As the stockpile decreases in size, the role of science, technology and engineering in deterrence will increase in importance."

Secretary Steven Chu June 2010

Our science-based strategy can sustain the deterrent without nuclear testing

Key elements

- Experimental science – providing validation and discovery
- Underlying science – R&D informing our models and solving problems
- Modeling and simulation – predicting weapons performance and safety
- Materials science-understanding materials performance in extreme regimes
- Manufacturing – sustaining current stockpile and provide capability to build the future stockpile
- Infrastructure – supporting all the above

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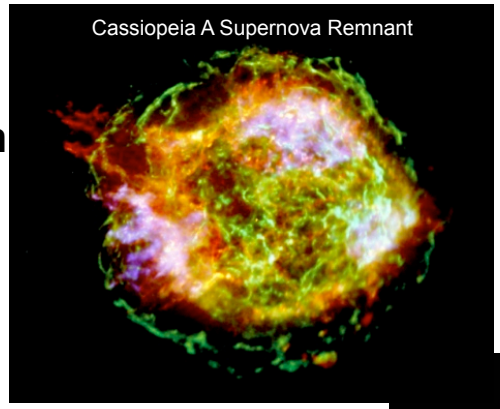
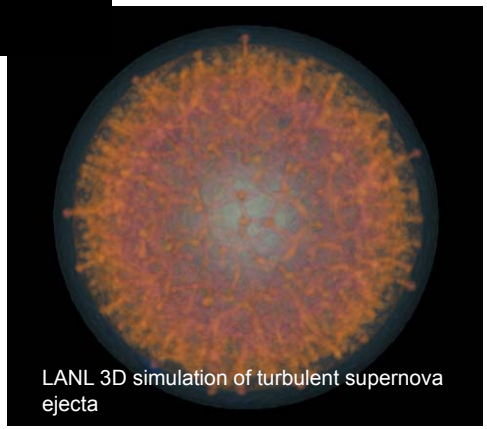
LDRD allows LANL to explore cutting edge research for which we are uniquely qualified to maintain excellence in all mission areas

Supernova light curves

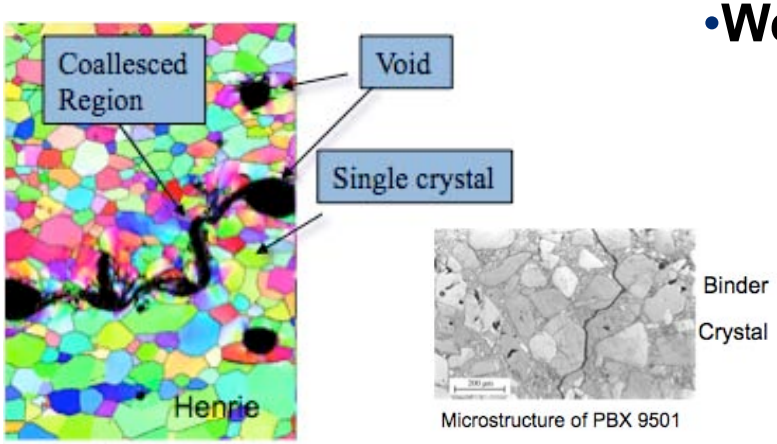
- These light curve studies benefitted from core weapons program resources:
  - Super-computing (Roadrunner)
  - Computational Methods
  - Physics models
- These LDRD funded studies provided the following benefits to the core weapons program:
  - Enhancing LANL radiation flow expertise
  - Advancing computer science
  - Providing opportunity for peer review of our capabilities
  - Recruiting and retaining new staff


Cassiopeia A Supernova Remnant


LANL 3D simulation of turbulent supernova ejecta

Through this effort, we showed the academic community that an integrated treatment of the stellar surroundings is critical

Understanding materials in extreme environments are key to LANL's weapons program success in the future



- **Current Stockpile**
  - Prediction of materials lifetime & failure
- **Rebuild & Lifetime Extension**
  - Materials 'by design' rather than re-learning old processes
- **Weapon performance**
  - Effects of microscale materials properties on dynamic performance for key physics

MATERIALS MATTER

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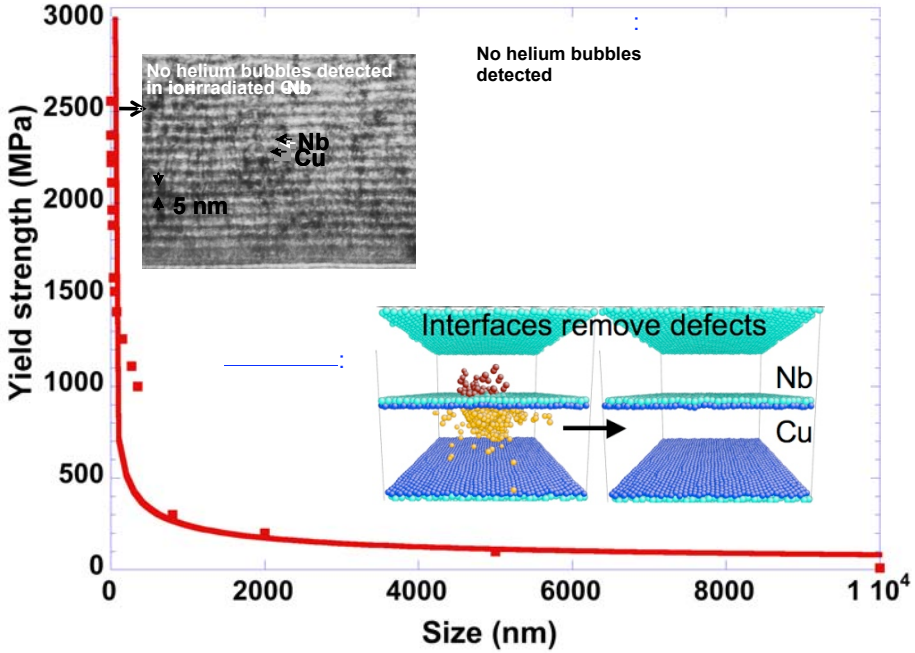
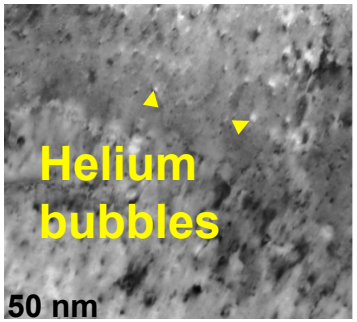
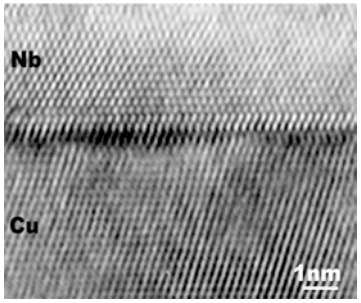
Nanoscale materials synthesis and advanced simulation is yielding transformational advances in materials behavior with broad applications

Initially funded by LDRD, LANL researchers discovered new mechanisms for substantially increasing materials strength and radiation resistance





Pure Cu



5 nm layer thickness
Cu-Nb multilayer

CMIME
Center for Materials at Irradiation and Mechanical Extremes

Energy Frontier Research Center ($19M)
funded by DOE at LANL

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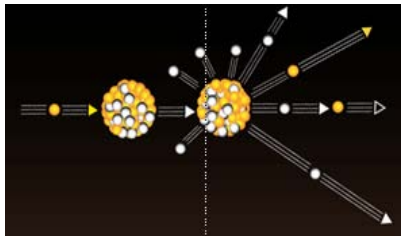
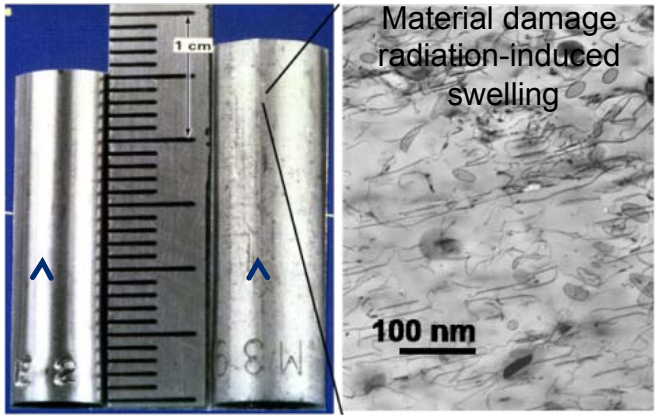
Materials behavior limits the performance of advanced energy systems needed for energy independence

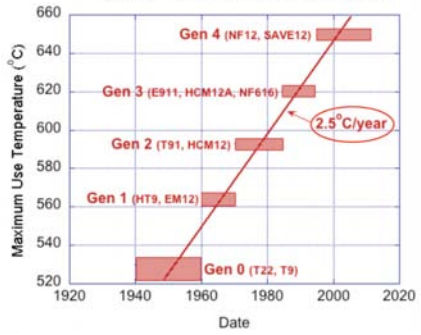
•Maximum operating temperature of reactor materials has only increased a few degrees per year since the 1950s due to a lack of predictive understanding of materials damage





Non-irradiated part

Radiated part



Higher performing materials can increase operating temperature leading to:

•more efficient fuel use

•reducing the number of reactors

•reducing the amount of waste produced to meet our clean energy need

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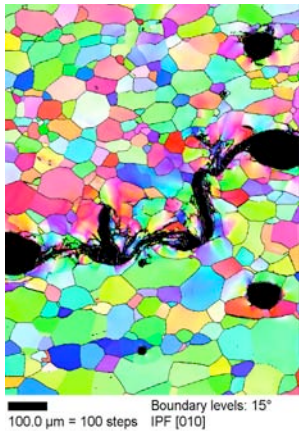
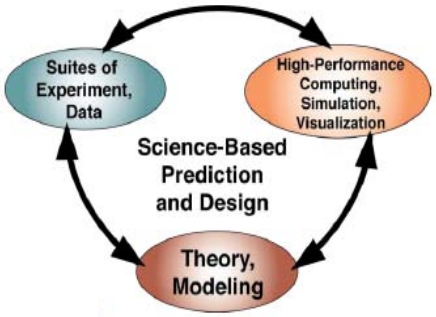
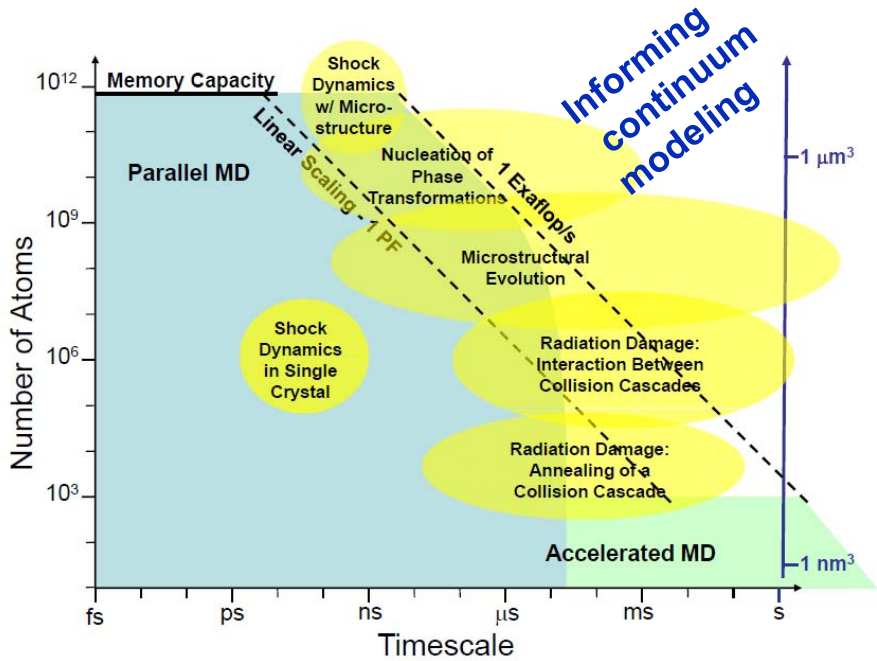
NNSA

Exascale computing, experimental tools with unprecedented resolution, and modeling put us on the verge of accessing critical phenomena at the meso (micron) scale

Significant breakthroughs are possible due to emerging advances in theory, computation, and experiment of materials microstructure







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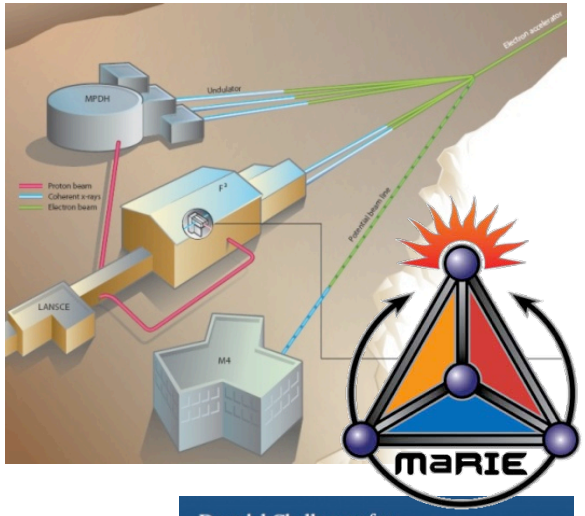
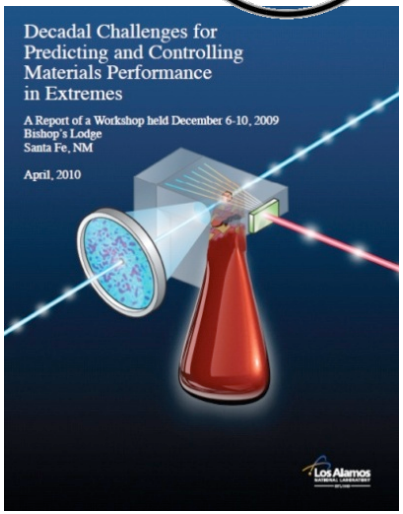
Materials research on the brink of a new era of science-traditional approach of observation and validation of performance is replaced by prediction and control of materials functionality

- **MaRIE builds on unique LANL capabilities to provide unique experimental tools needed to realize this vision**
- **In situ, dynamic measurements of real materials**
  - *Scattering & imaging simultaneously*
- **In extreme environments**
  - *Dynamic & irradiation extremes*
- **Coupled to directed synthesis via predictive theory**
  - *Materials design & discovery*





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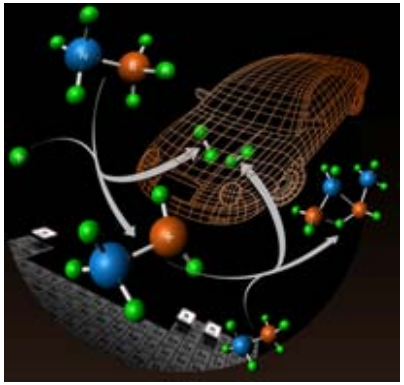
Exascale computing and understanding materials at the meso scale benefits ALL LANL missions

- **Exascale computing and advancing materials science to the meso scale is a significant scientific challenge that will require breakthrough discoveries in many fields over many years**
  - LDRD research will be essential in these efforts
- **Transitioning to exascale computing and MaRIE will allow LANL to:**
  - Enhance ability to surveill and assess the Nation's nuclear deterrent
  - Provide long term options for future LEPs
  - Design technologies to better protect electric transmission infrastructure from attack
  - Create novel materials for industrial applications—economic competitiveness
  - Develop technologies to enhance energy production/transmission and storage



- **People: Our most important resource and recognized worldwide**
  - **Collaborative work environment sustains scientific inquiry and supports Laboratory missions—weapons, nonproliferation, and basic science**
  - **Areas of expertise: nuclear design and engineering, supercomputing, materials science, complex experimentation, and manufacturing science**
  - **MacArthur, R&D 100, E. O. Lawrence, APS fellows, members of National Academy of Sciences**

Sixty-six years of scientific and technical excellence solving the nation's security challenges

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- **BACKUPS**

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